

Cacti with maximum Kirchhoff index

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Abstract: The concept of resistance distance was first proposed by Klein and Randić. The Kirchhoff index $Kf(G)$ of a graph G is the sum of resistance distance between all pairs of vertices in G . A connected graph G is called a cactus if each block of G is either an edge or a cycle. Let $Cat(n; t)$ be the set of connected cacti possessing n vertices and t cycles, where $0 \leq t \leq \lfloor \frac{n-1}{2} \rfloor$. In this paper, the maximum kirchhoff index of cacti are characterized, as well as the corresponding extremal graph.

Keywords: Cactus; Kirchhoff index; Resistance distance.

1 Introduction

Topological indices and graph invariants based on the distances between the vertices of a graph are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds [1].

All graphs considered in this paper will be finite, loopless, and contain no multiple edges. Let G be a connected graph with vertex set $V(G)$, and edge set $E(G)$. The ordinary distance between u and v , denoted by $d_G(u, v)$, is the number of edges in a shortest path joining u and v in G . For other undefined notations and terminology from graph theory, the readers are referred to [2]. The famous Wiener index [3] is equals to the sum of distances between all pairs of vertices, that is,

$$W(G) = \sum_{i < j} d_G(v_i, v_j).$$

On the basis of electrical network theory, Klein and Randić [4] posed a new distance function named resistance distance in 1993. They viewed G as an electrical network N by replacing each edge of G with a unit resistor. The term resistance distance was used for the physical interpretation [5]: one imagines unit resistors on each edge of a connected graph G with vertices v_1, v_2, \dots, v_n and takes the resistance distance between vertices v_i and v_j of G to be the effective resistance between vertices v_i and v_j , denoted by $R_G(v_i, v_j)$. This new kind of distance between vertices of a graph was diffusely studied in detail [1, 4, 6 - 12].

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Analogous to the Wiener index, the Kirchhoff index [4] is defined as

$$Kf(G) = \sum_{i < j} R_G(v_i, v_j).$$

The Kirchhoff index of graphs as well as its application in chemistry attracts broad attention since it was put forward. Much work has been done to compute the Kirchhoff index of some classes of graphs, or give bounds for the Kirchhoff index of graphs and characterize extremal graphs. In unicyclic graphs extremal with respect to the Kirchhoff index were determined in [13, 14]. Deng also studied the extremal Kirchhoff index of a class of unicyclic graphs [15] and graphs with a given number of cut edges [16]. The extremal graphs with given matching number, connectivity, and minimal Kirchhoff index were characterized by Zhou in [17]. Wang [5] determined the first three minimal Kirchhoff indices among cacti. For further details and additional references, the readers may refer to [18 - 22].

Let G be a connected graph, and $\deg_G(v)$ be the degree of a vertex v in G . The longest path of G , considered in this paper, is a path with the largest resistance distance. A pendent vertex of G is a vertex of degree 1. Let $P_k = r_1 r_2 \cdots r_k (k \geq 2)$ be a path of G with distinct vertices r_1, r_2, \dots, r_k and assume that $\deg_G(r_1) \geq 3, \deg_G(r_2) = \cdots = \deg_G(r_{k-1}) = 2$, then P_k is called a pendent path of length $k - 1$ at r_1 in G if $\deg_G(r_k) = 1$, and P_k is called a internal path if $\deg_G(r_k) \geq 3$ [23]. We suppose that G_1 and G_2 are two disjoint connected graphs with $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$. Let $(G, u) = (G_1, u_1) \oplus (G_2, u_2)$ denote the graph G created by the coalescence of u_1, u_2 , and denote the new common vertex by u . We refer to this procedure from G_1 and G_2 to G as an identification operation [24].

A connected graph G is called a *cactus* if each block of G is either an edge or a cycle. Denote by $Cat(n; t)$ the set of connected cacti possessing n vertices and t cycles, where $0 \leq t \leq \lfloor \frac{n-1}{2} \rfloor$. We call G a *star cactus* if all blocks share a common cut vertex. A *chain cactus* is a cactus graph G if each block of it has at most two cut vertices and each cut vertex is shared by exactly two blocks. Any chain cactus with at least two blocks contains exactly two blocks that have only one cut-vertex. Such blocks are called *terminal blocks* [23]. The cactus graph has many applications in real life problems, especially in radio communication system [25].

In this paper, the maximum kirchhoff index of cacti are characterized, as well as the corresponding extremal graph. The paper is organized as follows. In Section 2 we propose some useful graph operations changing the kirchhoff indices of graphs, we also cite some basic results used in the following sections. In Section 3 we find the extremal cacti with the maximum Kirchhoff and give explicit precise for the maximum kirchhoff index of cacti.

2 Preliminaries

Lemma 2.1 [4] Let x be a cut vertex of a connected graph G , and let a and b be vertices occurring in different components which arise upon deletion of x . Then $R_G(a, b) = R_G(a, x) + R_G(x, b)$.

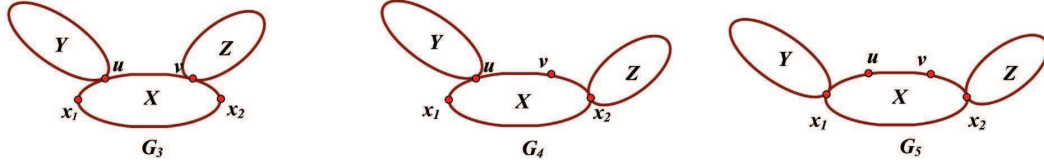


Fig. 1. The graphs of Lemma 2.3

Lemma 2.2 [5] Let G_1 and G_2 be connected graphs. If we identify any vertex, say x_1 , of G_1 with any other vertex, say x_2 , of G_2 as a new common vertex x , and we obtain a new graph G , then

$$Kf(G) = Kf(G_1) + Kf(G_2) + n_1 Kf_{x_2}(G_2) + n_2 Kf_{x_1}(G_1),$$

where $Kf_{x_i}(G_i) = \sum_{y_i \in G_i} R_{G_i}(x_i, y_i)$, and $n_i = |V(G_i)| - 1$ for $i = 1, 2$.

Lemma 2.3 Let X , Y and Z be connected graphs. Suppose that a is a vertex of Y , b is a vertex of Z , x_1 and x_2 are two endpoints of a longest path in X , u and v are two vertices of X satisfying $0 \leq R_X(x_1, u) \leq R_X(x_1, v) \leq R_X(x_1, x_2)$. Let G_3 be the graph constructed from X , Y , Z by identifying a with u and b with v , G_4 be formed from X , Y , Z by identifying a with u and b with x_2 , G_5 be created from X , Y , Z by identifying a with x_1 and b with x_2 , as displayed in Fig. 1. Then

- (1) when $Kf_v(X) \leq Kf_{x_2}(X)$, we have $Kf(G_3) < Kf(G_4)$;
- (2) when $Kf_u(X) \leq Kf_{x_1}(X)$, we have $Kf(G_4) < Kf(G_5)$.

Proof. (1) For convenience, we denote $x \in V(G)$ by $x \in G$. By the definition of kirchhoff index, one can get that

$$\begin{aligned} Kf(G_3) &= \sum_{x,y \in Y-a} R_Y(x,y) + \sum_{x,y \in Z-b} R_Z(x,y) + \sum_{x,y \in X} R_X(x,y) + \sum_{\substack{x \in X \\ y \in Y-a}} R_{G_3}(x,y) \\ &+ \sum_{\substack{x \in X \\ y \in Z-b}} R_{G_3}(x,y) + \sum_{\substack{x \in Y-a \\ y \in Z-b}} R_{G_3}(x,y) \end{aligned}$$

and

$$\begin{aligned} Kf(G_4) &= \sum_{x,y \in Y-a} R_Y(x,y) + \sum_{x,y \in Z-b} R_Z(x,y) + \sum_{x,y \in X} R_X(x,y) + \sum_{\substack{x \in X \\ y \in Y-a}} R_{G_4}(x,y) \\ &+ \sum_{\substack{x \in X \\ y \in Z-b}} R_{G_4}(x,y) + \sum_{\substack{x \in Y-a \\ y \in Z-b}} R_{G_4}(x,y). \end{aligned}$$

Note that, for $x \in X, y \in Z - b$,

$$R_{G_4}(x,y) = R_Z(y,b) + R_X(x,x_2) \quad \text{and} \quad R_{G_3}(x,y) = R_Z(y,b) + R_X(x,v).$$

Then

$$R_{G_4}(x,y) - R_{G_3}(x,y) = R_X(x,x_2) - R_X(x,v).$$

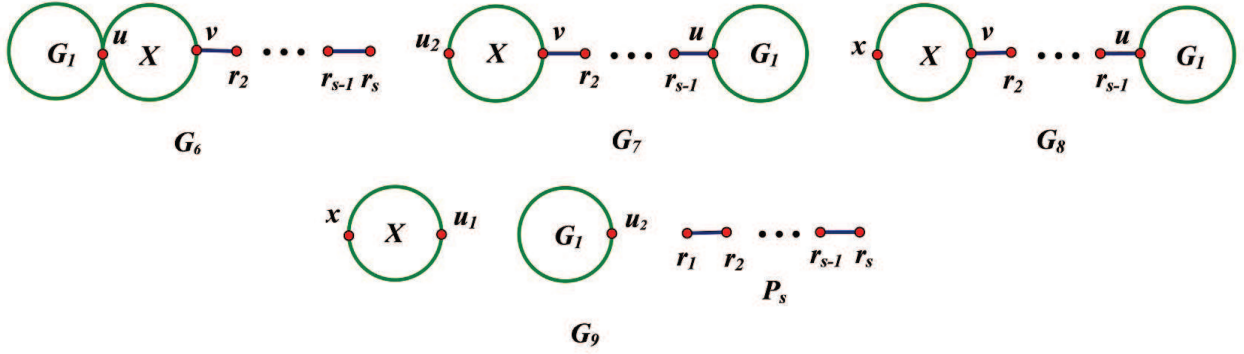


Fig. 2. The graphs of Lemma 2.4

For $x \in Y - a, y \in Z - b$,

$$R_{G_4}(x, y) - R_{G_3}(x, y) = R_X(u, x_2) - R_X(u, v) > 0.$$

Hence, when $Kf_{x_2}(X) \geq Kf_v(X)$, it follows that

$$\begin{aligned} Kf(G_4) - Kf(G_3) &= \sum_{\substack{x \in X \\ y \in Z - b}} (R_{G_4}(x, y) - R_{G_3}(x, y)) + \sum_{\substack{x \in Y - a \\ y \in Z - b}} (R_{G_4}(x, y) - R_{G_3}(x, y)) \\ &= \sum_{\substack{x \in X \\ y \in Z - b}} (R_X(x, x_2) - R_X(x, v)) + \sum_{\substack{x \in Y - a \\ y \in Z - b}} (R_X(u, x_2) - R_X(u, v)) \\ &> (|Z| - 1)(Kf_{x_2}(X) - Kf_v(X)) \\ &\geq 0. \end{aligned}$$

(2) In a similar way to prove (1), we can prove (2). (For reference, please see appendix.)

Then the proof of this lemma is complete. \square

The procedure of transformation from G_3 to G_4 is called an operation I. Let G_1 and X be two cacti not isomorphic to paths, u_2 and x are two end vertices of a longest path in X . Then G_6 and G_7 are obtained by identification operation as follows:

$$\begin{aligned} (M, v) &= (X, x) \oplus (P_s, r_1), \\ (G_6, u) &= (M, u_2) \oplus (G_1, u_1), \quad (G_7, u) = (M, r_s) \oplus (G_1, u_1). \end{aligned}$$

G_8 is constructed by attaching G_1 and X to r_1, r_s of P_s , respectively. That is $(N, v) = (X, u_2) \oplus (P_s, r_1)$ and $(G_8, u) = (N, r_s) \oplus (G_1, u_1)$. Let G_9 be the group of G_1, X and P_s . We call the process from G_6 to G_7 or G_8 an operation II. G_6, G_7, G_8 and G_9 are drawn in Fig. 2.

Lemma 2.4 Let G_6, G_7 and G_8 be three cacti defined above. For arbitrary connected graph X containing at least one cycle, we have

$$Kf(G_6) < Kf(G_7) \quad \text{or} \quad Kf(G_6) < Kf(G_8).$$

Proof. Firstly, we prove $Kf(G_6) < Kf(G_7)$. By Lemma 2.2,

$$\begin{aligned} Kf(G_6) &= Kf(G_1) + Kf(M) + (|M| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{u_2}(M), \\ Kf(G_7) &= Kf(G_1) + Kf(M) + (|M| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{r_s}(M). \end{aligned}$$

It can be calculated that

$$\begin{aligned} Kf_{u_2}(M) &= Kf_{u_2}(X) + Kf_{u_2}(P_s) - R(u_2, x) = Kf_{u_2}(X) + (s - 1)R(u_2, x) + Kf_{r_1}(P_s), \\ Kf_{r_s}(M) &= Kf_{r_s}(P_s) + Kf_{r_s}(X) - R(r_1, r_s) = Kf_{r_s}(P_s) + (s - 1)(|X| - 1) + Kf_x(X). \end{aligned}$$

Then we have

$$\begin{aligned} Kf_{r_s}(M) - Kf_{u_2}(M) &= (s - 1)(|X| - 1 - R(u_2, x)) + Kf_x(X) - Kf_{u_2}(X), \\ Kf(G_7) - Kf(G_6) &= (|G_1| - 1)((s - 1)(|X| - 1 - R(u_2, x)) + Kf_x(X) - Kf_{u_2}(X)). \end{aligned}$$

Note that

$$|X| > R(u_2, x) + 1,$$

So we have $Kf(G_6) < Kf(G_7)$ when $Kf_x(X) \geq Kf_{u_2}(X)$. Similarly, we can get that $Kf(G_6) < Kf(G_8)$ when $Kf_{u_2}(X) \geq Kf_x(X)$. (For reference, please see appendix.) From the above arguments, the result follows. \square

Lemma 2.5 [5] Let u_1 be a vertex of a connected graph G_1 and w, x be two vertices of a cycle C_k ($k > 3$) with the largest $R(w, x)$. G^* is a cactus depicted in Fig. 3, $(G^{**}, u) = (G_1, u_1) \oplus (C_k, w)$. Then $Kf(G^*) < Kf(G^{**})$.

As is shown in Fig. 3, G_{10} is a k -vertex graph obtained by identifying one vertex from C_3 with one pendent vertex from P_{k-2} , while G_{11} is obtained by identification operation $:(G_{11}, u) = (G_1, u_1) \oplus (G_{10}, r_{k-2})$.

Lemma 2.6 Let G^{**} and G_{11} be two cacti illustrated in Fig. 3. The procedure from G^{**} to G_{11} is called an operation III. Then $Kf(G^{**}) < Kf(G_{11})$.

Proof. By Lemma 2.2,

$$\begin{aligned} Kf(G^{**}) &= Kf(G_1) + Kf(C_k) + (|C_k| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_w(C_k), \\ Kf(G_{11}) &= Kf(G_1) + Kf(G_{10}) + (|G_{10}| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{r_{k-2}}(G_{10}). \end{aligned}$$

Therefore,

$$\begin{aligned} Kf(G_{11}) - Kf(G^{**}) &= Kf(G_{10}) - Kf(C_k) + (|G_1| - 1)(Kf_{r_{k-2}}(G_{10}) - Kf_w(C_k)) \\ &\quad + (|G_{10}| - |C_k|)Kf_{u_1}(G_1). \end{aligned}$$

Also by Lemma 2.2, we have

$$Kf(G_{10}) = Kf(C_3) + Kf(P_{k-2}) + (|C_3| - 1)Kf_{r_1}(P_{k-2}) + (|P_{k-2}| - 1)Kf_{r_1}(C_3).$$

It can be calculated that

$$\begin{aligned} Kf_{u_2}(G_{11}) &= Kf_{u_1}(G_1) + (|G_1| - 1)R(u, u_2) + Kf_{u_2}(G_{10}), \\ Kf_x(G^{**}) &= Kf_{u_1}(G_1) + (|G_1| - 1)R(u, x) + Kf_x(C_k). \end{aligned}$$

Then,

$$\begin{aligned} Kf_{u_2}(G_{11}) - Kf_x(G^{**}) &= Kf_{u_2}(G_{10}) - Kf_x(C_k) + (|G_1| - 1)(R(u, u_2) - R(u, x)) \\ &> Kf_{u_2}(G_{10}) - Kf_x(C_k). \end{aligned}$$

Recall that, $Kf(C_l) = \frac{l^3-l}{12}$, $Kf_v(C_l) = \frac{l^2-1}{6}$ and $Kf(P_m) = \frac{m^3-m}{6}$. Then one can have

$$\begin{aligned} Kf_{u_2}(G_{10}) &= \frac{1}{6}(3k^2 - 11k + 14), \\ Kf_x(C_k) &= \frac{1}{6}(k^2 - 1). \end{aligned}$$

Therefore, since $k > 3$, it follows that

$$\begin{aligned} Kf(G_{13}) - Kf(G_{12}) &> (|G_2| - 1)(Kf_{u_2}(G_{11}) - Kf_x(G^{**})) \\ &> (Kf_{u_2}(G_{10}) - Kf_x(C_k)) \\ &= \frac{1}{6}(2k - 5)(k - 3) \\ &> 0. \end{aligned}$$

This completes the proof. \square

Lemma 2.8 Let G_{13} be the graph defined in Lemma 2.7 and G_{14} be the cactus of Fig. 5. Assume a is the vertex of C_3 with $\deg_{G_{13}}(a) = 2$ in G_{13} . The process from G_{14} to G_{13} is referred to as an operation V. Therefore, if $|G_1| \leq |G_2|$, then $Kf(G_{13}) \leq Kf(G_{14})$. Moreover, the equality holds if and only if $|G_1| = |G_2|$.

Proof. Let G'_{10} and G'_{11} be connected graphs as indicated in Fig. 5. It is easy to obtain that

$$\begin{aligned} Kf(G_{13}) &= Kf(G_{11}) + Kf(G_2) + (|G_{11}| - 1)Kf_{v_1}(G_2) + (|G_2| - 1)Kf_{u_2}(G_{11}), \\ Kf(G_{14}) &= Kf(G'_{11}) + Kf(G_1) + (|G'_{11}| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{r_{k-2}}(G'_{11}). \end{aligned}$$

Furthermore,

$$\begin{aligned} Kf(G_{11}) &= Kf(G_1) + Kf(G_{10}) + (|G_{10}| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{r_{k-2}}(G_{10}), \\ Kf(G'_{11}) &= Kf(G_2) + Kf(G'_{10}) + (|G'_{10}| - 1)Kf_{v_1}(G_2) + (|G_2| - 1)Kf_{u_2}(G'_{10}). \end{aligned}$$

Therefore,

$$\begin{aligned} Kf(G_{14}) - Kf(G_{13}) &= (|G_1| - 1)(Kf_{r_{k-2}}(G'_{11}) - Kf_{r_{k-2}}(G_{10})) \\ &+ (|G_2| - 1)(Kf_{u_2}(G'_{10}) - Kf_{u_2}(G_{11})) \\ &+ (|G'_{11}| - |G_{10}|)Kf_{u_1}(G_1) + (|G'_{10}| - |G_{11}|)Kf_{v_1}(G_2). \end{aligned}$$

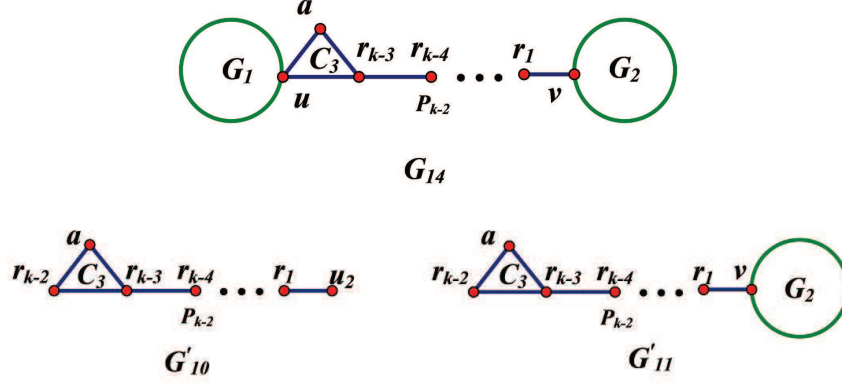


Fig. 5. The graphs of Lemma 2.8

Note that,

$$\begin{aligned} Kf_{r_{k-2}}(G_{10}) &= Kf_{u_2}(G'_{10}) = \frac{1}{6}(3k^2 - 3k - 10), \\ Kf_{u_2}(G_{10}) &= Kf_{r_{k-2}}(G'_{10}) = \frac{1}{6}(3k^2 - 11k + 14) \end{aligned}$$

and

$$\begin{aligned} Kf_{u_2}(G_{11}) &= Kf_{u_1}(G_1) + (|G_1| - 1)R(u, u_2) + Kf_{u_2}(G_{10}), \\ Kf_{r_{k-2}}(G'_{11}) &= Kf_{v_1}(G_2) + (|G_2| - 1)R(v_1, r_{k-2}) + Kf_{r_{k-2}}(G'_{10}). \end{aligned}$$

Thus,

$$\begin{aligned} Kf(G_{14}) - Kf(G_{13}) &= \left(\frac{4}{3}k - 4\right)(|G_2| - |G_1|) - (|G_2| + |G_{10}| - |G'_{11}| - 1)Kf_{u_1}(G_1) \\ &\quad + (|G_1| + |G'_{10}| - |G_{11}| - 1)Kf_{v_1}(G_2). \end{aligned}$$

Obviously,

$$\begin{aligned} (|G_2| + |G_{10}| - |G'_{11}| - 1) &= (|G_2| + |G'_{10}| - |G'_{11}| - 1) = 0, \\ (|G_1| + |G'_{10}| - |G_{11}| - 1) &= (|G_1| + |G_{10}| - |G_{11}| - 1) = 0. \end{aligned}$$

So we can get that

$$Kf(G_{14}) - Kf(G_{13}) = \left(\frac{4}{3}k - 4\right)(|G_2| - |G_1|).$$

This implies that $Kf(G_{13}) \leq Kf(G_{14})$ when $|G_1| \leq |G_2|$ and the equality holds if and only if $|G_1| = |G_2|$. Thus the conclusion holds. \square

Lemma 2.3 to Lemma 2.8 indicate that the operations from I to V can lead to increasing the $Kf(G)$ of a cactus G .

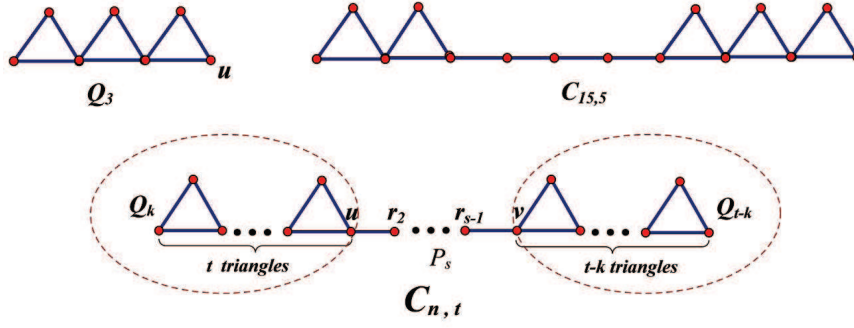


Fig. 6. The examples of Q_k and $C_{n,t}$

3 Main results

In this section we characterize the extremal cacti with the largest Kirchhoff in $Cat(n; t)$. Assume that Q_k is a chain cactus consisting of $k = \lfloor \frac{t}{2} \rfloor$ triangles. u and v , satisfying $\deg(u) = \deg(v) = 2$, are two vertices from the terminal blocks of Q_k and Q_{t-k} , respectively. Let $C_{n,t}$ (see Fig. 6) be another chain cactus obtained from P_s , Q_k and Q_{t-k} by identifying u with r_1 , v with r_s . That is

$$(F, u) = (Q_k, u) \oplus (P_s, r_1), \quad (C_{n,t}, v) = (F, r_s) \oplus (Q_{t-k}, v).$$

At first, we develop mathematical formulae describing Kf -values of $C_{n,t}$. By the definitions of kirchhoff index, it is easy to check that

$$Kf_u(Q_k) = \frac{2}{3}(k^2 + k).$$

Through accurate calculation, we arrive at

$$Kf_{r_s}(P_s) = \frac{1}{2}(s-1)s \quad \text{and} \quad Kf(P_s) = \frac{1}{6}(s^3 - s).$$

While by Lemma 2.2 and use of appropriate superposition computation, one can easily obtain that

$$\begin{aligned} Kf(Q_k) &= Kf(Q_1) + Kf(Q_{k-1}) + 2Kf_u(Q_{k-1}) + (|Q_{k-1}| - 1)Kf_u(Q_1) \\ &= \frac{2}{9}(2k^3 + 6k^2 + k). \end{aligned}$$

Similarly, for F , we can get that

$$\begin{aligned} Kf_{r_s}(F) &= Kf_{r_s}(P_s) + Kf_u(Q_k) + (|Q_k| - 1)(s-1) \\ &= \frac{1}{2}(s^2 - s) + \frac{2}{3}(k^2 + k) + 2k(s-1) \end{aligned}$$

and

$$\begin{aligned} Kf(F) &= Kf(Q_k) + Kf(P_s) + (|Q_k| - 1)Kf_{r_s}(P_s) + (|P_s| - 1)Kf_u(Q_k) \\ &= \frac{2}{9}(2k^3 + 3k^2 - 2k) + \frac{1}{6}(s^3 - s) + \frac{1}{3}ks(2k + 3s - 1). \end{aligned}$$

So, for $C_{n,t}$, we have

$$Kf(C_{n,t}) = Kf(F) + Kf(Q_{t-k}) + (|F| - 1)Kf_v(Q_{t-k}) + (|Q_{t-k}| - 1)Kf_{r_s}(F).$$

$$\text{Note that, } n = 2t + s \text{ and } k = \lfloor \frac{t}{2} \rfloor = \begin{cases} \frac{t}{2}, & \text{if } t \text{ is even;} \\ \frac{t-1}{2}, & \text{if } t \text{ is odd.} \end{cases}$$

Thus, by the definition of kirchhoff index and suitable precise computation, it can be calculated that

$$Kf(C_{n,t}) = \begin{cases} \frac{1}{18}(3n^3 - 3n - 12nt^2 - 6nt + 8t^3 + 12t^2 - 2t), & \text{if } t \text{ is even;} \\ \frac{1}{18}(3n^3 - 15n - 12nt^2 - 6nt + 8t^3 + 12t^2 + 22t + 12), & \text{if } t \text{ is odd.} \end{cases}$$

Next, we demonstrate that $C_{n,t}$ is the extremal cacti with the maximum Kf . For $Cat(n; t)$, $Cat(n; 0)$ is the set of all trees and $Cat(n; 1)$ is the set of unicyclic graphs. Their extremal graphs are $Cat(n; 0) = P_n$ and $Cat(n; 1)$, respectively. So we suppose that $n \geq 5$ and $t \geq 2$.

Theorem 3.1 $G \in Cat(n; t) - \{C_{n,t}\}$ for $n \geq 5$ and $t \geq 2$, then

$$Kf(G) < Kf(C_{n,t}).$$

Proof. The proof contains the following four steps.

Firstly, suppose that G is a connected graph, but not isomorphic to chain cactus, then a chain cactus H_1 is created by repeated applications of the operation I described in Lemma 2.3. By Lemma 2.3, it follows that

$$Kf(G) < Kf(H_1).$$

Obviously, all the cut vertices of H_1 are in a longest path.

In the second step, our goal is convert pendent paths into internal paths. At present, H_1 consists of at most two pendent paths, which are only possibly fused to the first and last cycles, respectively. Assume that H_1 has one pendent path P_t or two. Without loss of generality, one can suppose that P_t is attached to the first cycle in H_1 , then P_t can be transformed into internal path by operation II defined in Lemma 2.4. We denote the new graph by H'_1 . From Lemma 2.4, one can easily conclude that

$$Kf(H_1) < Kf(H'_1).$$

In a similar way, we can have the same results if there is another pendent path attached to the last cycle. Thus, there is no pendent path in the newly constructed graph H_2 .

Now, it comes to the third step. In this step, we will use two operations mentioned above. Let C_l ($l > 3$) be any cycle of H_2 . If C_l contains only one cut vertex, then use operation III established in Lemma 2.6 ; If C_l contains two cut vertices, then apply operation IV described in Lemma 2.7 to it. After finite times transformations in this step, we rapidly construct a cactus H_3 , in which every cycle is triangle. According to Lemmas 2.5, 2.6 and 2.7, we arrive at

$$Kf(H_2) < Kf(H_3).$$

Finally, let $H_3 \not\cong C_{n,t}$. Suppose that H_3 contains only one internal path which is not between Q_k and Q_{t-k} . We use operation V defined in Lemma 2.8 for appropriate times, then we have

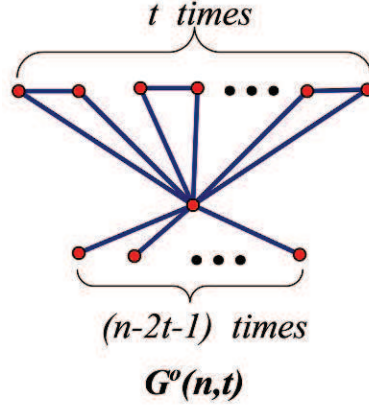


Fig. 7. Cactus with the minimum Kirchhoff index

the chain cactus $C_{n,t}$. If there are more than one internal path in H_3 , fuse every internal path into a unique internal path connecting Q_k and Q_{t-k} by operation V, then $C_{n,t}$ is also created. we have

$$Kf(H_3) < Kf(C_{n,t})$$

based on Lemma 2.8.

Therefore, by the four steps above, we constructed chain cactus $C_{n,t}$. Since G is not isomorphic to chain cactus, it is not difficult to demonstrate that $G \not\cong C_{n,t}$, thus

$$Kf(G) < Kf(C_{n,t}).$$

□

In the end of this section, we give upper and lower bounds of Kf -value of a cactus. In [5], the minimum Kirchhoff index and the corresponding extremal graph, denote by $G^0(n, t)$ (see Fig. 7), are presented by Wang and Hua. Combining the results given by them, we arrive at the following proposition.

Proposition 3.2 Let G be any n -vertex cactus different from $C_{n,t}$ and $G^0(n, t)$, then

$$Kf(G^0(n, t)) < Kf(G) < Kf(C_{n,t}).$$

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Appendix

Proof of Lemma 2.3(2). For convenience, we denote $x \in V(G)$ by $x \in G$. By the definition of kirchhoff index, one can get that

$$\begin{aligned} Kf(G_5) &= \sum_{x,y \in Y-a} R_Y(x,y) + \sum_{x,y \in Z-b} R_Z(x,y) + \sum_{x,y \in X} R_X(x,y) + \sum_{\substack{x \in X \\ y \in Y-a}} R_{G_5}(x,y) \\ &+ \sum_{\substack{x \in X \\ y \in Z-b}} R_{G_5}(x,y) + \sum_{\substack{x \in Y-a \\ y \in Z-b}} R_{G_5}(x,y), \end{aligned}$$

and

$$\begin{aligned} Kf(G_4) &= \sum_{x,y \in Y-a} R_Y(x,y) + \sum_{x,y \in Z-b} R_Z(x,y) + \sum_{x,y \in X} R_X(x,y) + \sum_{\substack{x \in X \\ y \in Y-a}} R_{G_4}(x,y) \\ &+ \sum_{\substack{x \in X \\ y \in Z-b}} R_{G_4}(x,y) + \sum_{\substack{x \in Y-a \\ y \in Z-b}} R_{G_4}(x,y). \end{aligned}$$

Note that, for $x \in X, y \in Y - a$,

$$R_{G_5}(x,y) = R_Y(y,a) + R_X(x,x_1) \quad \text{and} \quad R_{G_4}(x,y) = R_Y(y,a) + R_X(x,u).$$

Then

$$R_{G_5}(x,y) - R_{G_4}(x,y) = R_X(x,x_1) - R_X(x,u).$$

For $x \in Y - a, y \in Z - b$,

$$R_{G_5}(x,y) - R_{G_4}(x,y) = R_X(x_1,x_2) - R_X(u,x_2) > 0.$$

Hence, when $Kf_{x_1}(X) \geq Kf_u(X)$, it follows that

$$\begin{aligned} Kf(G_5) - Kf(G_4) &= \sum_{\substack{x \in X \\ y \in Y-a}} (R_{G_5}(x,y) - R_{G_4}(x,y)) + \sum_{\substack{x \in Y-a \\ y \in Z-b}} (R_{G_5}(x,y) - R_{G_4}(x,y)) \\ &= \sum_{\substack{x \in X \\ y \in Y-a}} (R_X(x,x_1) - R_X(x,u)) + \sum_{\substack{x \in Y-a \\ y \in Z-b}} (R_X(x_1,x_2) - R_X(u,x_2)) \\ &> (|Y| - 1)(Kf_{x_1}(X) - Kf_u(X)) \\ &\geq 0. \end{aligned}$$

□

Proof of Lemma 2.4(2). Here, we prove $Kf(G_6) < Kf(G_8)$. By Lemma 2.2,

$$\begin{aligned} Kf(G_6) &= Kf(G_1) + Kf(M) + (|M| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{u_2}(M), \\ Kf(G_8) &= Kf(G_1) + Kf(N) + (|N| - 1)Kf_{u_1}(G_1) + (|G_1| - 1)Kf_{r_s}(N). \end{aligned}$$

It can be calculated that

$$\begin{aligned} Kf(M) &= Kf(X) + Kf(P_s) + (s-1)Kf_x(X) + (|X| - 1)Kf_{r_1}(P_s), \\ Kf(N) &= Kf(X) + Kf(P_s) + (s-1)Kf_{u_2}(X) + (|X| - 1)Kf_{r_1}(P_s) \end{aligned}$$

and

$$\begin{aligned} Kf_{u_2}(M) &= Kf_{u_2}(X) + Kf_{u_2}(P_s) - R(u_2, x) = Kf_{u_2}(X) + (s-1)R(u_2, x) + Kf_{r_1}(P_s); \\ Kf_{r_s}(N) &= Kf_{r_s}(P_s) + Kf_{r_s}(X) - R(r_1, r_s) = Kf_{u_2}(X) + (s-1)(|X| - 1) + Kf_{r_s}(P_s). \end{aligned}$$

Note that

$$|X| > R(u_2, x) + 1,$$

Then we have

$$Kf_{r_s}(N) - Kf_{u_2}(M) = (s-1)(|X| - 1 - R(u_2, x)) > 0.$$

Hence

$$\begin{aligned} Kf(G_8) - Kf(G_6) &= Kf(N) - Kf(M) + (|G_1| - 1)(Kf_{r_s}(N) - Kf_{u_2}(M)) \\ &= (s-1)(Kf_{u_2}(X) - Kf_x(X)) + (|G_1| - 1)(Kf_{r_s}(N) - Kf_{u_2}(M)) \\ &> (s-1)(Kf_{u_2}(X) - Kf_x(X)). \end{aligned}$$

So we have $Kf(G_6) < Kf(G_8)$ when $Kf_{u_2}(X) \geq Kf_x(X)$. □